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Strong terahertz conductance of graphene nanoribbons under a magnetic field

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We demonstrate that the optical response of graphene nanoribbons in the terahertz to far-infrared regime can be significantly enhanced and tuned by an applied magnetic field. The dependence of the threshold frequency on the magnetic field is studied. The ribbons with the strongest terahertz conductance under a magnetic field are those with one-dimensional massless Dirac Fermion energy dispersion. For a given ribbon, there exists an optimal field under which the conductance resonance can occur at the lowest frequency. © *2008 American Institute of Physics*.
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Recent progress in isolating single sheets of graphite[1–4] has sparked interest in graphene-based nanoelectronics. Experiments have already demonstrated anticipated physics such as electron-hole symmetry and the half-integer quantum Hall effect,[2,3] finite conductivity at zero charge-carrier concentration,[2] the strong suppression of weak localization,[5–8] etc. By further confining the electrons in the graphene plane, one can obtain one-dimensional structures which we refer to as graphene nanoribbons (GNRs). It has been suggested that these GNRs could be used as field-effect transistors.[9,10] These properties promise building blocks for technological applications in molecular electronic and optoelectronic devices.

Low-energy electronic states of graphene with a linear dispersion at the corner of Brillioun zone are described by the "relativistic" massless Dirac equation. This relativistic kinematical description of graphene is confirmed in quantum Hall studies[11] and gives us theoretical insight into exotic transport,[12] magnetic correlation,[13–15] and dielectric properties[16] observed in this material. The linear energy dispersion of two-dimensional electrons leads to other unique transport and optical properties in graphene.[17]

The optical response of graphene is rather weak with the absorption around a few percent in the far-infrared (FIR) and visible range.[18–20] The weak response in the terahertz/FIR regime is mainly due to two fundamental reasons: (1) the density of states vanishes near the Fermi energy and (2) the interband transition amplitude is small. The optical response of graphene increases as frequency increases and reaches a cusplike maximum for $\hbar\omega=2t$, where t is the nearest neighbor hopping bandwidth in grapheme.[18] The optical response at selective frequencies can be enhanced with the use of GNRs.[21,22] Several types of zigzag and armchair ribbons have been studied recently. Optical conductance exhibits strong peaks at frequencies corresponding to resonant interband absorption in given ribbons. In these nanoribbons, however, no optical response was detected and the nearly universal conductance in the visible range is totally suppressed making them transparent in this frequency range. For all zigzag and armchair ribbons, the low frequency conductance is zero and the first response peak appears at a frequency corresponding to the allowed transition with the lowest energy gap.

In this letter, we study the optical conductance of GNRs in the important frequency band of terahertz to FIR. We show that the large threshold frequency that prevented terahertz and FIR response in ribbons can be reduced to a much lower value, making these GNRs active in the terahertz and FIR regime. Therefore controlled terahertz radiation can be achieved in GNRs through the applied magnetic field.

It is commonly accepted that the transport and optical properties in graphene are mainly due to the π electrons of carbon atoms. A nanoribbon can be constructed from a chain of m connected carbon hexagons,[23] and by translating this chain by the translational vector $\mathbf{T}=q\mathbf{a}+\mathbf{b}$, $(q<m)$. Therefore a nanoribbon is indexed by a set of two integers p and q with $p=m-q$. In the nearest neighbor hopping tight-binding model, the Hamiltonian of a ribbon is given as,[23]

$$H=\sum_i \varepsilon_i c_i^\dagger c_i+\sum_{i,j} t_{ij} c_i^\dagger c_j, \tag{1}$$

where ε_i is the site energy, t_{ij} is the hopping bandwidth, and $c_i^\dagger(c_i)$ is the creation (annihilation) operator of the π electron at site i. The presence of a ribbon edge will modify both the site energy and hopping bandwidth for the edge electrons. In this work, we shall neglect these effects as they are quite small. We take the transfer energy to be t (around 3.03 eV) between all the nearest neighbor sites and otherwise to be 0. The eigenfunctions are given as $\psi_{kj}=\xi_j e^{iky}$, which satisfy $H\psi_{kj}=\varepsilon_{kj}\psi_{kj}$, where ξ_j denotes the jth eigenvector of the Hamiltonian with $(j=1,2,3\ldots 2N)$. Here N is the number of carbon layers in a ribbon, $N=p+1$ for zigzag ribbon and $p+3$ for armchair ribbons.

In order to calculate the conductance of ribbons using the Kubo formula, we first write the form of the current operator,

$$J_x=e\frac{\partial H}{\partial(\hbar k_x)},\quad J_y=e\frac{\partial H}{\partial(\hbar k_y)}, \tag{2}$$

where we have introduced an infinitesimal transverse vector potential A_x and rewrite the Harper equation for solving J_x. By introducing the field operator $\hat{\psi}(x,y)=\Sigma_{k,j}\xi_j e^{iky}c_{kj}$, the

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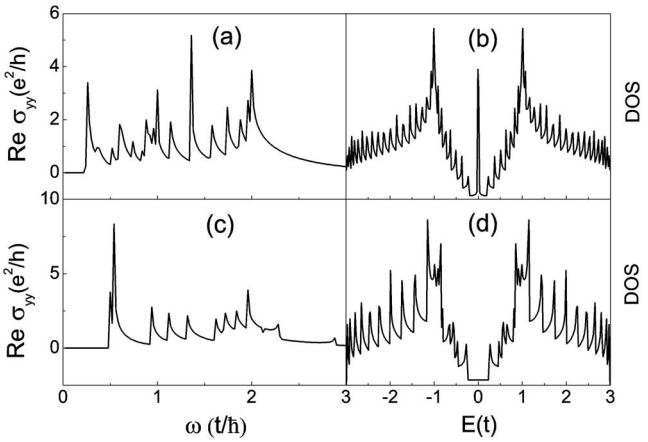

FIG. 1. Optical conductance and the corresponding DOS for zigzag and armchair ribbons under zero magnetic field. (a) and (b) are for a (19,0) zigzag ribbon. (c) and (d) are for a (17,1) armchair. The chemical potential $\mu=0$.

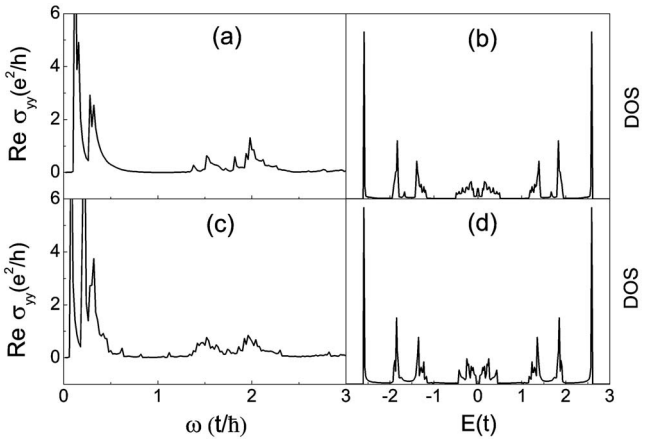

FIG. 2. Optical conductance and the corresponding DOS for zigzag and armchair ribbons in a strong magnetic flux $f=0.25$. (a) and (b) are for a (19,0) zigzag ribbon, (c) and (d) are for a (17,1) armchair ribbon. The chemical potential $\mu=0$.

current operator can be expressed in the second quantization notation,

$$\hat{J}_\mu = \int dy \hat{\psi}^\dagger(x,y) J_\mu \hat{\psi}(x,y) = \sum_{kjj'} J^\mu_{jj'} c^\dagger_{kj} c_{kj'}, \tag{3}$$

with $J^\mu_{jj'}=\xi^\dagger_j J_\mu \xi_{j'}$ and $\mu=x,y$. According to the Kubo formula, the optical conductance is found as

$$G_{\mu\nu}(\omega) = -\frac{1}{i\omega}\sum_{kjj'} J^\mu_{jj'} J^\nu_{j'j} \frac{f_{kj}-f_{kj'}}{\hbar\omega+\epsilon_{kj}-\epsilon_{kj'}+i\delta}, \tag{4}$$

where f_{kj} and $f_{kj'}$ are Fermi distribution functions and δ is positive infinitesimal. As the transverse average of the conductance, the optical conductivity reads $\sigma_{\mu\nu}(\omega)=G_{\mu\nu}(\omega)/W$, where W is the physical width of the ribbon. For zigzag ribbons, $W=(3p+1)a/2$, and for armchair ribbons, $W=(\sqrt{3}a/2)(p+2)$.

The optical conductance of typical zigzag and armchair ribbons under zero magnetic field is shown in Fig. 1. The characteristics of zigzag and armchair ribbons have been analyzed previously.[21,22] The selection rule for allowed transitions has been determined for both types of ribbon. The main feature is a series of van Hove type absorption peaks at frequencies corresponding to the allowed interband transitions. The edge states of GNRs play an important role in the optical absorption. They are involved in many of the absorption peaks within the optical range and have no contribution to the absorption peaks beyond the optical range. For all ribbons, there exists a threshold frequency (ω_0) below which the optical conductance is zero. For metallic ribbons, the optical conductance at low frequency is virtually zero, although the density of states at zero energy is quite large. This is because the dipole matrix element due to transitions between the highest valance band and lowest conduction band vanishes. As a result, GNRs are not good candidates for optoelectronics applications such as sensors operating at low frequencies. The threshold frequency decreases as width of ribbons increases. For the zigzag ribbon, we can see that the threshold frequency corresponds to the transition between the states whose energies are located at the middle peak and the states whose energies are located at the first right peak from the middle peak. It is known that the middle peak is caused by the edge states which are characteristic to zigzag ribbons.[13] There exist states near the energy $E=0$ for all the zigzag ribbons, which make all the zigzag ribbons metallic. As we can see, the peak at $\omega=2$ in the optical conductance curve stems from the transitions from the states near the peak $E=-1$ to those near the peak $E=1$ in density of states (DOS) curve. Similarly, the peak at $\omega=1$ is attributed to both the transition from the peak $E=-1$ to the peak $E=0$ and the transition from the peak $E=0$ to the peak $E=1$. Moreover, the conductance depends strongly on the position of the chemical potential. In general the optical absorption in the low frequency region decreases and the threshold frequency increases as the chemical potential increases. For the armchair ribbon, the threshold frequency corresponds to the allowed transition from the second valence band to the second conduction band.

To achieve a strong optical response in a nanoribbon in the visible and low frequency range, it is necessary to lift the strict selection rules that forbid the dipole interband transitions at lower energies. This can be achieved by introducing finite disorder scattering.[24,25] For intrinsic graphene, the selection rules can be modified to allow terahertz/FIR transitions by applying a perpendicular magnetic field. When a magnetic field is introduced,

$$E\psi_i = \sum_j t_{ij} e^{i\gamma_{ij}} \psi_j, \tag{5}$$

where $\gamma_{ij}=(2\pi/\phi_0)\int_i^j \mathbf{A}\cdot d\mathbf{l}$ is the magnetic phase factor, with $\phi_0=hc/e$ being the magnetic flux quantum. The Schrödinger equation for the A and B sublattice can be obtained.[15] The B-field modifies the energy dispersions and changes the size of the bandgap, induces the semiconductor-metal transition and generates the partial flat bands.[26] As the magnetic field increases such that the cyclotron radius is smaller compared to the ribbon width, the Landau levels are developed. This will allow absorption by direct transitions between the magnetic subbands. Figure 2 shows the optical conductance of zigzag and armchair ribbon in a strong magnetic field $f=0.25$, where $f=3\sqrt{3}Ba^2/2\phi_0$ is the magnetic flux through the hexagon in units of ϕ_0. The Landau levels can be seen clearly in the DOS curves. The absorption peaks are attributed to the transition between two of these Landau levels.

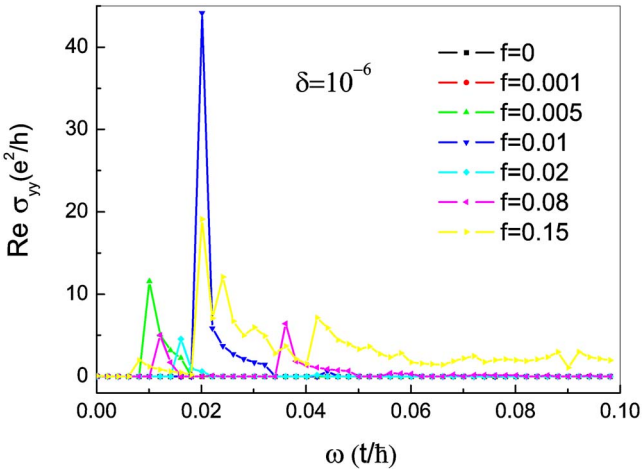

FIG. 3. (Color online) Optical conductance of a (17,1) armchair ribbon under various magnetic fields. The chemical potential $\mu=0$.

which is similar to the case of a graphene sheet.[27] The threshold frequencies are dramatically reduced and a strong optical response can occur at low frequencies. At $f=0.25$, the ω_0 decreases by a factor of 3 for a (19,0) zigzag ribbon and by an order of magnitude for a (17,1) armchair ribbon. For the (17,1) armchair ribbon, the first conductance peak now occurs around the 30 THz region. For a given tube, the position and intensity of the first conductance resonance can be tuned by varying the magnetic field. For the (17,1) tube, the conductance resonance can occur at $\omega=7$ THz under $f=0.005$. By increasing the B field to $f=0.01$, ω_0 increases to 15 THz while the resonance intensity increases by a factor of 4. The variation of the threshold frequency with the field is shown in Fig. 3. At high frequencies, the optical conductance for a zigzag ribbon and that for an armchair ribbon tend to be the same. This is because the Landau levels are well developed in the high energy region but not in the low energy region where the Landau levels are strongly influenced by the edge.

The strongest magnetic enhancement of terahertz conductance occurs in ribbons with one-dimensional massless Dirac Fermion energy dispersions at Γ point. All $(3n\text{-}1,1)$ armchair ribbons and a selective chiral ribbons belong to this class. The nearly zero dipole matrix elements in these ribbons in the absence of a B field are now finite due to the formation of the magnetic subbands. For zigzag ribbons, the magnetic enhancement is much weak. This is due to that in all zigzag ribbons, the conduction band touches the valence band at the zone boundary, not the zone center.

Our result of strong terahertz and FIR optical conductance for GNRs should significantly enhance the potential application of graphene structures as optoelectronic materials in this important frequency band. FIR photodetectors and possible terahertz emitters can be developed by using these nanoribbons.

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